A Critical Review Of The Drag Force On A Sphere In The Transition Flow Regime

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Abstract. Improvements in micro-fabrication techniques are enabling Micro-Electro-Mechanical-Systems to be constructed with sub-micron feature sizes. At this scale, even at standard atmospheric conditions, the flow is in the transition regime. This paper considers the range $0.1 < Kn < 1$, where non-equilibrium effects can be appreciable, and specifically illustrates problems involving non-planar surfaces by analyzing the drag force for low speed, incompressible flow past an unconfined microsphere. A critical comparison is made between experimental data, analytical solutions derived from kinetic theory, Grad's thirteen-moment equations, and the Navier-Stokes equations with first- and second-order treatment of the slip boundary. The results, even for this simple geometry, highlight major problems in predicting the drag in the transition flow regime for non-kinetic schemes.

INTRODUCTION

Developments in Micro-Electro-Mechanical-Systems (MEMS) continue to show that fluid mechanics in small-scale devices can differ significantly from those encountered in the macroscopic world. For example, surface and viscous effects will govern the flow behavior and gas flows, in particular, will show a significant departure from the continuum regime. Micro-channel experiments performed by Harley *et al.* [1] and Arkilic *et al.* [2] on low speed gas flows have demonstrated that the mass flow rates cannot be predicted by traditional continuum analyses.

The continuum hypothesis of the Navier-Stokes equations can only be applied when the mean free path of the molecules is much less than the characteristic dimension of the flow domain. When the mean free path of the gas approaches the characteristic length scale of the device, the flow will start to display a variety of non-continuum or rarefaction effects, including the breakdown of the traditional no-slip boundary condition.

The mean free path can be defined as

$$\lambda = \frac{\mu}{\phi \, \rho \, \overline{c}} \, , \tag{1}$$

where μ is the viscosity of the gas, ρ is the density, $\overline{c}$ is the mean velocity of the gas molecules and ϕ is a constant that depends upon the theory employed. It can be shown from kinetic theory [3] that, for the hard sphere model, ϕ takes the value 0.491. However, hydrodynamic models commonly assume ϕ is 0.5 (Gad-el-Hak [4]).

The ratio between the mean free path, λ, and the characteristic dimension of the flow geometry, L_c, is known as the Knudsen number, *Kn*:

$$Kn = \frac{\lambda}{L_c} \, . \tag{2}$$

The validity of the Navier-Stokes equations can be gauged from the Knudsen number, which determines the degree of rarefaction of a gas. The gradual change of a flow from continuum to free molecular can be broadly classified as follows:

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$$Kn < 0.01 \qquad \text{Continuum flow}$$
$$0.01 < Kn < 0.1 \qquad \text{Slip flow}$$
$$0.1 < Kn < O(10) \qquad \text{Transition flow} \tag{3}$$
$$Kn > O(10) \qquad \text{Free molecular flow.}$$

For $Kn < 0.01$, it is generally accepted that the Navier-Stokes equations, in conjunction with the no-slip boundary condition, provide an adequate description of the flow. However, it has been suggested by Gad-el-Hak [4] that rarefaction effects are discernible at Knudsen numbers as low as $Kn = 0.001$. Following ideas proposed by Maxwell, the Navier-Stokes equations can be extended into the slip-flow regime provided the Knudsen number, Kn, is less than 0.1 (Schaaf and Chambré [5]). However, improvements in micro-fabrication techniques are enabling systems to be constructed with sub-micron feature dimensions. At this scale, even at standard atmospheric conditions, the flow will depart further from equilibrium and will enter the transition flow regime ($0.1 < Kn < 10$).

In practice, a typical MEMS device will have to operate over a range of Knudsen numbers but of particular interest is the range $0.1 < Kn < 1$, where non-equilibrium effects start to be significant. For example, air flowing at SATP in a device with a characteristic dimension of 100 nm would have a Knudsen number of approximately 0.7. Under such conditions, the traditional first-order treatment of the slip-flow boundary in conjunction with the Navier-Stokes equations is no longer appropriate. There have been several attempts to extend slip-flow analysis into the transition regime by modifying the boundary conditions to be locally second-order in Knudsen number [6,7] *viz.*

$$u_{slip} = \pm A_1 \, \lambda \, \frac{\partial u}{\partial n} - A_2 \, \lambda^2 \, \frac{\partial^2 u}{\partial n^2} \, . \tag{4}$$

For planar surfaces, this approach has met with some success, as demonstrated by Maurer *et al*. [8] in a study of the mass flow rates through rectangular ducts. However, there is still no real agreement between the theoretical and experimental values for A_2 and it is believed that the disparity is caused by neglecting Knudsen layer effects [9].

An alternative approach to modeling flows in the transition regime is to use methods that are globally second-order accurate, or higher, in Knudsen number, such as the Burnett equations or Grad's thirteen moment equations. These approaches, however, introduce significant complexity and non-linearity making numerical stability a critical issue. Moreover, the applicability of these methods to complex geometries requires much further investigation. This paper will present results that will illustrate serious concerns when non-planar boundaries are involved. To illustrate the problem, the drag force on an unconfined microsphere is considered because a critical comparison can be made between experimental results [10-13], analytical solutions derived from kinetic theory [14,15], Grad's thirteen-moment equations [16], and the Navier-Stokes equations with first- and second-order treatment of the slip boundary. The results, even for this relatively simple non-planar problem, highlight significant problems for higher-order schemes in predicting the drag in the transition flow regime.

CREEPING FLOW PAST AN UNCONFINED SPHERE

Gas microflows are generally associated with low speed incompressible flows. In the absence of inertia, Stokes demonstrated that the total drag force due to the flow of a Newtonian fluid around a sphere is given by

$$F = 6\pi\mu a U \, , \tag{5}$$

where a is the radius of the sphere and U is the unbounded fluid velocity. For this particular problem, there are several analytical solutions covering a range of Knudsen numbers that are supported by good experimental data acquired over many years of research.

Experimental Results For Flow Around Spherical Particles

One of the first experiments to determine the drag on a spherical particle was performed by Millikan [10] as part of his landmark oil drop experiment. Millikan measured the drag force on oil droplets as they settled through air over a range of Knudsen numbers up to 96 and showed that Stokes' drag equation (5) had to be modified at higher Knudsen numbers. He proposed an empirical formula of the form

$$F = 6\pi\mu a U \left[1 + Kn \left(\alpha + \beta e^{-\gamma/Kn} \right) \right]^{-1} , \tag{6}$$

where α, β and γ are experimentally determined constants and Kn is the Knudsen number based on the radius of the sphere. Allen and Raabe [11] reviewed Millikan's experimental data using modern, more accurate physical constants and non-linear least-squares fitting techniques. The values obtained by re-analyzing Millikan's data are

$$\alpha = 1.155 \pm 0.008 \qquad \beta = 0.471 \pm 0.011 \qquad \gamma = 0.596 \pm 0.050 . \tag{7}$$

More recently, new experimental techniques have been used in an attempt to study Millikan's formula for different materials. In experiments performed by Allen and Raabe [12], three different types of solid particles (polystyrene latex-divinylbenzene, polyvinyltoluene and polystyrene latex) were used, over a range of Knudsen numbers from 0.03 to 7.2. The constants in Eq. (6) were determined to be

$$\alpha = 1.142 \pm 0.0024 \qquad \beta = 0.558 \pm 0.0024 \qquad \gamma = 0.999 \pm 0.0212 . \tag{8}$$

Hutchins *et al.* [13] measured the drag force on spherical polystyrene latex particles using a modulated dynamic light scattering technique; a technique fundamentally different to that used by Millikan or Allen and Raabe. The drag was measured for a range of Knudsen numbers from 0.06 to 500. The constants in Eq. (6) were found to be

$$\alpha = 1.231 \pm 0.0022 \qquad \beta = 0.470 \pm 0.0037 \qquad \gamma = 1.178 \pm 0.0091 . \tag{9}$$

Analytical Solution Derived From The Navier-Stokes Equations

For Knudsen numbers in the slip-flow regime, the tangential slip-velocity can be related to the shear stress, τ, by

$$\vec{u}_{slip} = \left(\frac{2-\sigma}{\sigma} \right) \frac{\lambda}{\mu} \vec{\tau} , \tag{10}$$

where σ is the Tangential Momentum Accommodation Coefficient (TMAC) and the arrow denotes a vector quantity. The TMAC can vary from zero (for specular reflection) up to unity (for complete or diffuse reflection). The boundary condition at the surface of the sphere can therefore be rewritten in polar (r, θ) co-ordinates as

$$u_\theta = \frac{2-\sigma}{\sigma} \lambda \left[\frac{\partial u_\theta}{\partial r} + \frac{1}{r} \frac{\partial u_r}{\partial \theta} - \frac{u_\theta}{r} \right]_{r=a} . \tag{11}$$

The analytical solution for the drag in the slip-flow regime is given by [17,18]

$$F = 6\pi\mu a U \left[\frac{1 + 2 \dfrac{2-\sigma}{\sigma} Kn}{1 + 3 \dfrac{2-\sigma}{\sigma} Kn} \right] , \tag{12}$$

which for $Kn \to 0$ recovers Stokes' original drag formula.

As previously discussed, the boundary conditions can be modified to be locally second-order accurate in Kn. A higher-order boundary condition appears desirable because the solution is dominated by gas-surface interactions. Following Lockerby *et al.* [19], the Burnett equations can be employed to derive higher-order boundary conditions for the Navier-Stokes equations. The complete solution is lengthy, so only the linear higher-order terms are considered in the present analysis. The linearized Maxwell-Burnett boundary condition can be written as

$$u_{slip} = \left(\frac{2-\sigma}{\sigma} \right) \frac{\lambda}{\mu} \vec{\tau}_x - \frac{3}{4} \left(\frac{\gamma-1}{\gamma} \right) \frac{Pr}{p} q_x^{MB} , \tag{13}$$

where Pr is the Prandtl number, γ is the ratio of specific heat capacities, and

$$q_x^{MB} = \frac{\mu^2}{8\rho} \left[(61-45\gamma) \frac{\partial^2 u}{\partial x^2} + (49-45\gamma) \frac{\partial^2 v}{\partial x \partial n} + (49-45\gamma) \frac{\partial^2 w}{\partial x \partial z} + 12 \frac{\partial^2 u}{\partial n^2} + 12 \frac{\partial^2 u}{\partial z^2} \right] , \tag{14}$$

where x and z are directions tangential to the boundary and perpendicular to each other and n is the direction normal to the surface. The velocities u, v and w are in the x, n and z directions, respectively.

Solving the Navier-Stokes equations using Eq. (13) at $r = a$ yields

$$F = 6\pi\mu aU \left[\frac{1 + 2\dfrac{2-\sigma}{\sigma} Kn}{1 + 3\dfrac{2-\sigma}{\sigma} Kn + \dfrac{9}{4\pi}\dfrac{(\gamma-1)}{\gamma} Pr\, Kn^2} \right]. \tag{15}$$

Analytical Solution Derived From Grad's Thirteen Moment Equations

Goldberg [16] derived a solution for flow around a sphere using Grad's thirteen moment equations, which are globally second-order accurate in *Kn*. Goldberg showed that the drag force can be expressed as

$$F = 6\pi\mu aU \left[\frac{\left(1 + \dfrac{15}{2}\dfrac{2-\alpha}{\alpha} Kn\right)\left(1 + 2\dfrac{2-\sigma}{\sigma} Kn\right) + \dfrac{6}{\pi} Kn^2}{\left(1 + \dfrac{15}{2}\dfrac{2-\alpha}{\alpha} Kn\right)\left(1 + 3\dfrac{2-\sigma}{\sigma} Kn\right) + \dfrac{9}{5\pi}\left(4 + 9\dfrac{2-\sigma}{\sigma} Kn\right) Kn^2} \right], \tag{16}$$

where α is the thermal accommodation coefficient.

Analytical Solutions Derived From Kinetic Theory

Epstein [20] showed that in the free-molecular regime, the drag force on a sphere for diffuse reflection is

$$F = \left(\frac{4}{3} + \frac{\pi}{6}\right)\pi\rho a^2 \bar{c} U . \tag{17}$$

Beresnev *et al*. [14] modified Eq. (17) to obtain an approximate expression over the entire Knudsen number regime:

$$F = 6\pi\mu aU \left(\frac{8+\pi}{18}\right)\frac{1}{0.619 + Kn}\left[1 + \frac{0.310 Kn}{0.785 + 1.152 Kn + Kn^2}\right]. \tag{18}$$

In the continuum limit, it can readily be shown that Eq. (18) tends to Stokes' drag formula.

Sone and Aoki [15] developed an alternative analytical solution that accounted for the Knudsen layer and thermal stress effects, which are neglected in classical slip-flow analyses. The drag was determined to be

$$F = 6\pi\mu aU \left[1 - 1.01619\left(\frac{2}{\sqrt{\pi}}\right) Kn + \left(0.5 + 0.2349\frac{K}{2K+1}\right)\left(\frac{2}{\sqrt{\pi}}\right)^2 Kn^2\right], \tag{19}$$

where $K = k_g / k_s$ represents the ratio of the thermal conductivities of the gas and solid particle, respectively.

RESULTS AND DISCUSSION

Figure 1 presents the non-dimensionalized drag force, ($F/6\pi\mu aU$), as a function of the Knudsen number, for creeping flow past an unconfined sphere. For consistency with kinetic models, the momentum and thermal accommodation coefficients, σ and α, have been taken as unity. As shown in Fig. 1, the analytical results derived from kinetic theory are in good agreement with the experimental data, well into the transition regime. In contrast, the results obtained from both Navier-Stokes and Grad's thirteen moment equations quickly deviate from the experimental results. For the case of no-slip, the Navier-Stokes equations predict a constant drag force irrespective of the Knudsen number. However, taking the hydrodynamic solution to first-order slip provides a dramatic improvement over the no-slip condition for very low Knudsen numbers. Moreover, for planar channels, Maurer *et al*. [8] found that extending the Navier-Stokes boundary treatment to be locally second-order in *Kn* significantly improved the predicted mass flow rates, up to a mean channel Knudsen number of 0.8. In stark contrast, the present results, for a non-planar surface, demonstrate that there is limited benefit to be gained by using a locally second-

order boundary treatment. Figure 1 also raises some serious concerns over the benefit of using globally second-order methods, such as Grad's thirteen moment equations, to extend into the transition flow regime.

The percentage error in the predicted drag force associated with the analytical models is presented in Fig. 2. The errors are shown relative to Millikan's re-analyzed experimental data [11]. It is evident that the kinetic models perform significantly better than Grad's thirteen moment solution and the hydrodynamic models. In particular, Beresnev's solution agrees very well with the experimental data up to $Kn = 1$ and, for a perfectly conducting solid particle ($K = 0$), Sone and Aoki's solution provides good agreement up to $Kn \approx 0.5$. However, all hydrodynamic models quickly depart from the experimental results and there appears to be no benefit to be gained by extending to Grad's method for this class of problem.
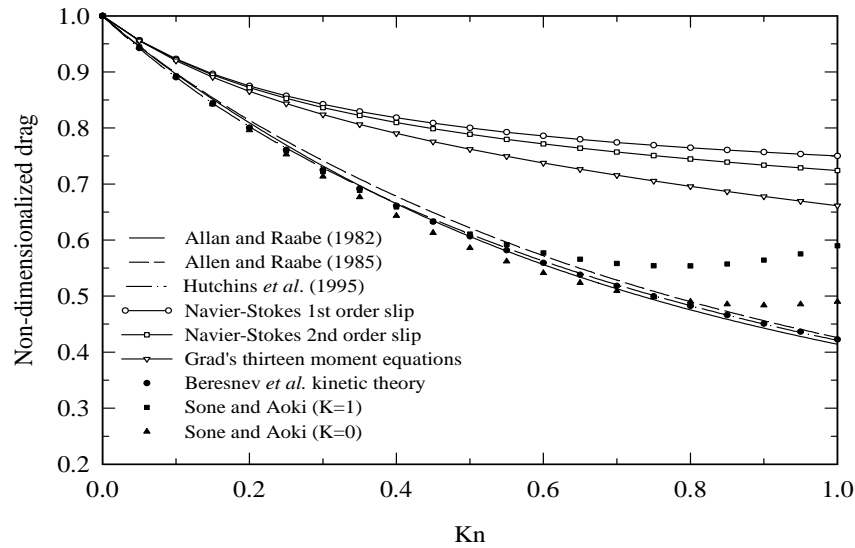

FIGURE 1. Non-dimensionalized drag as a function of Knudsen number for unconfined flow past a sphere.
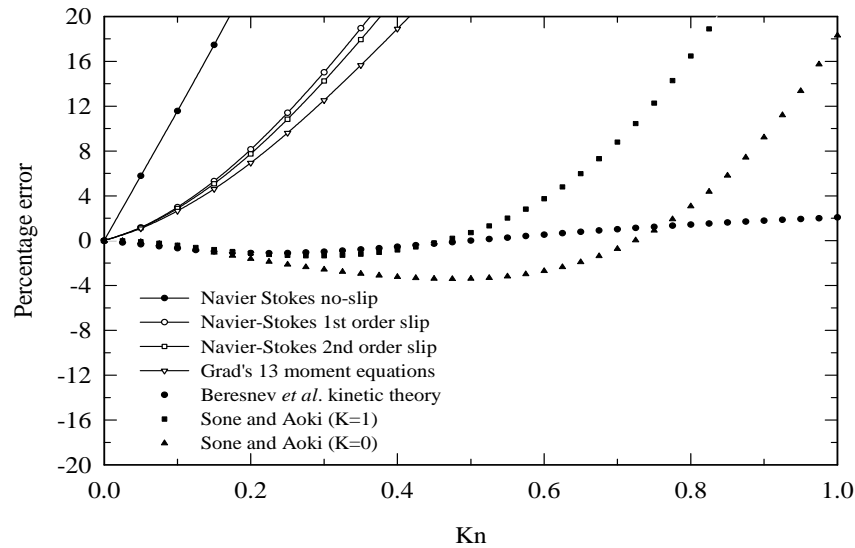

FIGURE 2. Percentage error in the drag force predicted by various hydrodynamic and kinetic models.

CONCLUDING REMARKS

Creeping flow past an unconfined microsphere has been investigated for Knudsen numbers up to unity. The study has focused on the behavior of rarefied flow over a curved surface. The results show that the drag force predicted by analytical models derived from kinetic theory agree well with experimental data. As expected, the inclusion of Maxwell's slip-flow boundary condition into the Navier-Stokes equations provides a significant improvement over the traditional no-slip approach. However, the implementation of a locally second-order boundary condition appears to offer no appreciable benefit over Maxwell's first-order approach. This is in contrast to results for planar channels, which indicate that a locally second-order boundary condition can extend the applicability of the Navier-Stokes equations into the transition regime. Of some concern, however, is the fact that Grad's thirteen moment equations, which are globally second-order in Knudsen number, offer little improvement over the Navier-Stokes slip-flow solution. It is probable that other higher-order approaches, such as the Burnett equations, may have similar limitations.

ACKNOWLEDGMENTS

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